Graphene-like massless Dirac fermions in Harper systems

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It is shown that systems described by Harper's equation exhibit a Dirac point at the center of the spectrum whenever the field parameter is a fraction of even denominator. The Dirac point is formed by the touching of two subbands, and the physics around such point is characterized by the relative field only, as if the latter were null at the reference value. Such behavior is consistent with the nesting property conjectured by Hofstadter, and its experimental verification would give support to such hypothesis as well as the Peierls-Onsager ansatz used to arrive at Harper's equation when crystalline electrons move in a uniform external magnetic field.

The relative simplicity with which graphene - carbon single layer sheets - may be made and handled in the laboratory has drawn much attention to the physics of massless Dirac particles.[1] In this material electrons moving in two dimensions (2D) near the Fermi level are subject to an effective energy dispersion law proportional to momentum rather than the usual momentum squared. The dynamics is similar to that of photons and phonons, except that in graphene the particles are charged fermions. They interact among themselves through the Coulomb force and with external electric and magnetic fields, which makes them amenable to a varied palette of experimental manipulation and possible applications.

In graphene carbon atoms are arranged in a two dimensional hexagonal lattice, obtained as the overlap of two identical triangular lattices displaced one respect to the other. As a result of the lattice symmetry the valence and conduction bands have two inequivalent degenerate points about which the dispersion is linear, the so called Dirac points.[2] The effect is absent in the square lattice. In this letter we show that for certain values of a perpendicular magnetic field the square lattice also supports a Dirac point where two subbands meet, however. Such special values are defined by a magnetic flux through the unit cell representing a fraction of flux quanta of even denominator. Furthermore, in the neighborhood of every one of these values Landau levels emerge from the Dirac point as they do from zero magnetic field in the hexagonal graphene lattice. At the reference field the massless Dirac particles behave as if there was no magnetic field and in its neighborhood, they appear to respond only to the difference field much as composite fermions do at major Landau level filling fractions of even denominator.[3] These results are a property of Harper's equation and therefore generic to all systems governed by such relation. Besides electrons in a square lattice and a perpendicular magnetic field the equation has appeared in several contexts, including the quantum Hall effect,[4,5] superconducting networks,[6] nonperiodic solids[7] and electrons in superlattices.[8]

The dynamics of Bloch electrons in a square lattice of lattice constant a and a perpendicular magnetic field B is governed by Harpers equation,[9]

$$f_{n+1} + f_{n-1} + 2\cos(2\pi\phi n + \nu) f_n = \varepsilon f_n, \tag{1}$$

where f_n is the amplitude of a Wannier state localized at site na along the x-axis, n an integer, ϕ is the magnetic flux traversing a plaquette in units of the flux quantum hc/e, $\nu = k_y a$ is the dimensionless momentum variable along the y-axis, and ε is the energy in units of the hopping integral t. The usual Landau gauge $\mathbf{A} = B(0, x, 0)$ is assumed. When the flux parameter is a rational $\phi = p/q$, p and q integers prime to each other, then the potential in equations (1) has period q and the set may be closed by selecting solutions with the property $f_{n+q} = exp(iq\mu) f_n$, $\mu = k_x a$. The condition for existence of solutions of the resulting q equations for the unknowns $f_1, f_2, ...f_q$ is that the determinant of the coefficients,

$$D(\varepsilon, \mu, \nu) = P_q(\varepsilon) - 2(\cos q\nu + \cos q\mu) + (-1)^{\frac{q}{2}} 4, \tag{2}$$

vanishes.[10] Here $P_q(\varepsilon)$ is a polynomial of even parity and degree q in ε, independent of the momentum variables ν and μ, and with the property $P_q(0) = 0$. The integer q has been assumed to be even. For each value of μ and ν Eq. 2) has q zeroes which, as these quantum numbers cover their range, span the q subbands present in the spectrum. If $q = 4s$, s a positive integer, one can verify that $\varepsilon = 0, \nu = \mu = 0$ is a solution of (2). Likewise, $\varepsilon = 0$, $\nu = \pm\pi/q$, $\mu = \pm\pi/q$ are solutions when $q = 2s$, s odd. Zero energy, the center of the field free band, is thus always in the spectrum. It corresponds to the edges of two separate subbands that meet at a single critical point in the Brillouin zone, its center if $q/2$ is even, and the four equivalent corners if odd. At this point two neighboring bands meet, never overlapping.[11]

That the dispersion near the center of the spectrum is linear in the magnitude of the momentum follows from the property $P_q(-\varepsilon) = P_q(\varepsilon)$ for all q even. Near zero energy one has $P_q(\varepsilon) \approx -(-1)^{\frac{q}{2}} A(p,q)\varepsilon^2$, where $A(1,2) = 1$,

$A(1,4) = 8$, $A(1,6) = 24$, $A(1,8) = 96 - 32\sqrt{2}$, $A(3,8) = 96 + 32\sqrt{2}$ ... are all positive constants.[12] The condition on the determinant (2) then simplifies to

$$A(p,q)\varepsilon^2 + 2(-1)^{\frac{q}{2}}(\cos q\nu + \cos q\mu) - 4 = 0. \tag{3}$$

For $q/2$ even this gives near the Brillouin zone center

$$\varepsilon = \pm C(p,q)\sqrt{\nu^2 + \mu^2}, \tag{4}$$

where $C(p,q) = qA(p,q)^{-1/2}$ is a magnetic field dependent velocity in units $ta/\hbar$. A similar relation is obtained near each Brillouin zone corner for $q/2$ odd, with the momentum measured respect to the appropriate zone corner. Figure 1(a) shows a Dirac point placed at the zone corners corresponding to $q = 2$, in which case form (3) is exact. Figure 1(b) is for $q = 4$ and exemplifies a Dirac point placed at the center of the zone. Specular reflection over the momentum plane gives the dispersion for negative energy, corresponding to holes. We note that although a 2D hexagonal crystal exhibits two inequivalent Dirac points at zero magnetic field, they are lost when the field is turned on except at special values of the flux of the form $\phi = n \pm 1/6$, n an integer or zero, where a single such critical point occurs.[13]

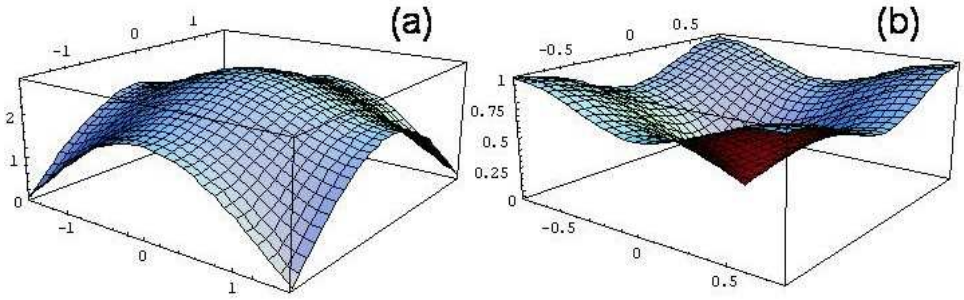

FIG. 1: Energy dispersion for (a) $q = 2$ and (b) $q = 4$. The energy (vertical axis) is in units of the band parameter t, while the perpendicular plane represents dimensionless momentum.

As shown by Hofstadter, the spectrum of Harpers equation has a recursive structure of nonoverlapping subbands arranged in such ways that, displayed over the fundamental cell $0 \leq \phi \leq 1$, resemble a butterfly with open wings.[14] He conjectured a nesting property that makes each subband in the spectrum a replica at some recursive level of the field-free band, about which a geometrically distorted version of the whole graph develops. One consequence is that, for instance, at $\phi' = \phi + \delta\phi$ a cyclotron frequency $\omega = q\delta\phi/\hbar g(\phi,\varepsilon)$ may be defined in the neighborhood of any subband pertaining to the spectrum at flux ϕ, where $g(\phi,\varepsilon)$ is the density of states at energy ε. Note that this expression scales as $\delta\phi$, as expected from the notion that the subband in question is a recursive replica of the field free parent band at $\phi = 0$.[15]

To study the special situation when two subbands touch at energy $\varepsilon = 0$ we take advantage of the effective hamiltonian formalism.[16] In this theory, the original problem of an electron moving in the presence of a square lattice potential and an external magnetic field B' in the neighborhood of a given subband belonging to the spectrum at field B, is replaced by the hamiltonian problem defined by

$$H_r = \varepsilon_r(\frac{1}{\hbar}[\mathbf{p} + \frac{e}{c}\Delta\mathbf{A}(\mathbf{r})], \phi), \tag{5}$$

where $\varepsilon_r(\mathbf{k},\phi)$ is the dispersion law in subband r and $\Delta\mathbf{A}(\mathbf{r}) = \delta B(0,x,0)$, with $\delta B = B' - B$. If the integer $r = 1, 2, ..., q$ labels the subbands in order of increasing energy then $\varepsilon_{q/2}$, $\varepsilon_{q/2+1}$ touch at zero energy, near which the dispersion obeys Eq. (3). In that neighborhood the dispersion is linear and the usual methods of quantum mechanics can be employed to obtain the associated spectrum and eigenfunctions.[17] The former is found to have the form

$$E_n = sgn(n)2qt\sqrt{\frac{\pi}{A(p,q)}|n\delta\phi|}, \tag{6}$$

where $\delta\phi = e\delta B a^2/hc$ is the flux traversing a unit cell, measured with respect to the reference value $\phi = p/q$, and $n = 0, \pm1, \pm2, ...$ is a Landau level index. Figure 2 shows this expression evaluated in the neighborhood of flux 1/2 up to $n = 4$ (solid lines), together with the associated spectrum given by roots of Eq. (2) at a few rational values of the flux in that neighborhood (dots). In the latter the Landau levels have a width and possibly internal structure,

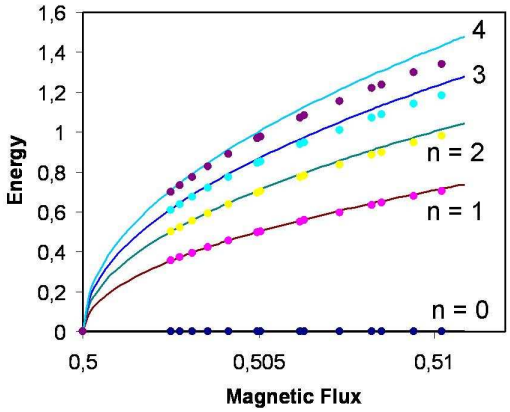

FIG. 2: Landau levels emerging from the Dirac point at 0.5 flux quanta per unit cell (solid lines), and solutions to Harper's equation in the same neighborhood (dots).

only that so narrow that it is not resolved in the scale of the figure. The agreement is excellent at low Landau levels, though it deteriorates slowly as the Landau index increases and the relative flux grows. The figure shows the positive quadrant only and it repeats for negative flux and negative energy, specularly reflected over the proper axes.

The number of states in each Landau level may be obtained from the gap labeling theorem, according to which the statistical weight of states below any gap in the spectrum is given by a continuous function of the field, of the form $W = M\phi + N$, with M, N integers.[18] The value $\varepsilon = 0$ divides the spectrum in two specularly symmetric halves, so at that energy $W = 1/2$. Using these two facts one readily finds that the number of states of any level in the Landau fan emerging from the Dirac point at flux $\phi = p/q$, q even, is simply $D = q\delta\phi$. For instance, for $\phi = 1/2$, the number of states per cell below a gap reaching the apex at $\varepsilon = 0$ has the form $W_N = (1 + 2N)\phi - N$, with N an integer. The number of states between two neighboring gaps is then $W_{N+1} - W_N = 2\phi - 1 = 2\delta\phi$, in accordance with the general result just described. The number of states grows linearly with the relative flux as it does for free 2D electrons in a magnetic field, yet the total number is q times larger. Inclusion of spin degeneracy is achieved through an additional factor of 2.

Landau levels are separated by sizable gaps traversing the energy versus field graph and meeting at the Dirac point. Here the gap labeling theorem yields the equation $s = Mp + 2sN$, $s = q/2$, which restricts the values of M to the set $M = s(2n + 1)$, n an integer. Since M may be identified with the dimensionless conductance,[4] in the neighborhood of a Dirac point at flux p/q one expects the inverse Hall resistance to be quantized according to

$$R_{xy}^{-1} = q(n + \frac{1}{2})\frac{e^2}{h}. \tag{7}$$

Because q is even, this quantity will always involve integer multiples of the quantum of conductance e^2/h even when the spin degeneracy is fully resolved. In the simple case $q = 2$ the sequence of multiples for electrons in the latter case is 1, 3, 5, ... but if the Zeeman energy is small the sequence is the same as that observed in graphene, e. g. 2, 6, 10, ...

The existence of Dirac points in Harper systems as shown, could play an important role in settling questions concerning such systems. One issue is the correctness of the Peierls-Onsager substitution method used in deriving Harpers equation from a tight binding field-free band, a yet unproven ansatz.[19,20] It works well in the semiclassical regime at small fields but its performance when the flux per cell approaches one flux quanta is largely unknown. Another issue is the nesting hypothesis used by Hofstadter to describe the recursivity of the spectrum, mentioned above.[14] Full experimental verification of the complex subband spectrum and associated dynamics predicted by Harper's equation would give strong support to both the Peierls-Onsager ansatz and the nesting hypothesis.

In order to enter the desired region of about one flux quantum per unit cell, experimentally unreachable magnetic fields in the order of 10^5 Tesla are required by ordinary atomic solids. However, artificial crystalline potentials with a lattice constant of about 10nm are possible, allowing to work in the few Tesla regime. Features of the Hofstadter butterfly have already been recognized as Landau level internal structure in the weak lattice potential limit.[21,22] As better samples become available it is hoped that the search of Shubnikov-de Hass oscillations and quantum Hall plateaus as one moves away from a Dirac point such as the one at $\phi = 1/2$ will give decisive information on the correctness of the Peierls-Onsager ansatz and the nesting hypothesis.

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